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# The fitting of Auxiliary Basis Sets to Electron Densities

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# The fitting of auxiliary basis sets to electron densities.

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The effect of changing the fitting requirement for the formation of an atom-centered auxiliary basis is studied. In this case the basis (contracted gaussian functions) directly represents the electron density (i.e. the diagonal element of the one-electron density matrix) and is used within the Kohn-Sham Density Functional Theory framework to approximate two-electron (Coulomb) contributions.

The cost in terms of accuracy in using a simple density fit is investigated and compared to that the standard electric field fit advocated by Dunlap.[2] Exploitation of both fitting requirements has been implemented within the MOLPRO[3] program.

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[2] B.I. Dunlap, J.W.D. Connolly and J.R. Sabin, "On First Row Diatomic Molecules and Local Density Models," *J. Chem. Phys.* **71**, 4993 (1979).

[3] MOLPRO is a package of ab initio programs written by H.-J. Werner and P. J. Knowles, with contributions from R. D. Amos, A. Bernhardsson, A. Berning, P. Celani, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, T. Korona, R. Lindh, A. W. Lloyd, S. J. McNicholas, F. R. Manby, W. Meyer, M. E. Mura, A. Nicklass, P. Palmieri, R. Pitzer, G. Rauhut, M. Schtz, H. Stoll, A. J. Stone, R. Tarroni, and T. Thorsteinsson.